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AUTHOR(S):

KITAMURA, Toyoyuki

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Solitons and Bound States of the Self-consistent Potential

Toyoyuki KITAMURA
Nagasaki Institute of Applied Science, Nagasaki 851-01, Japan

We have established a quantum field theory of phonons and phonon instability in crystals, amorphous solids and liquids from the view-point of the spontaneous breakdown of the symmetry starting with atoms interacting with each other in the harmonic potential approximation in the two band model:[1-12] An atom in the matter feels a harmonic potential. When an atom is excited from the ground state to the first excited state, a neighbouring atom drops from the first excited state to the ground state, and vice versa. Thus a particle-hole pair spreads over the matter. This collective excitation is called a phonon. In the nearest neighbour approximation and the random phase approximation, the structure of phonons is determined by the pair distribution function of atoms. In the disordered matter, energy spectrum of an atom has bands; there are gaps. The gaps ensure rigidity. The phonon life times originate from the energy bands of atoms; when a phonon merges in the continuum, the phonon has a finite life time. Phonon instability occurs when the gaps disappear.

Up to now, the interaction Hamiltonian is constructed as the coupling between two particle-hole pairs. Even in this interaction , the effect of nonlinearity is taken into account in the two ways: i) An essential point is that the interaction Hamiltonian is nonlinear by itself. It is represented by the two body interaction of atoms. Even within the two band model, we can carry out thermodynamical treatment and investigate life time of phonons and phonon instability. ii) In the multi-band model, a higher excited state wavefunction is represnted by a function of spatial derivatives on the ground state one. The partial integrations lead to the higher derivatives on the potential. In the conventional theory, the higher derivatives appear in an anharmonic potential. But in this case, a higher excited state modifies the structure of phonons at rather high temperatures.

However, the above-mentioned nonlinearity can not explain the existence of a soliton solution. It only explains the structure of phonons and phonon instability. This is because the interction Hamiltonian includes the couplings between only two particle-hole pairs. A particle-hole pair corresponds to a displacement of an atom from the equilibrium position of the atom; the displacement of an atom corresponds

to the spread of the wavefunction due to the excitation of the atom. In the coventional nonlinear theory, a soliton solution is derived from the interaction Hamiltonian with cubic or quartic relative displacements of atoms. Thus the interaction Hamiltonian should include three or more particle-hole pairs to derive a soliton solution.

The purpose of the present paper is to obtain the bound states due to the self-consistent potential induced by the extended objects (solitons).[13] We first derive a Heisenberg equation for phonon operators in nonlinear lattices taking into account higher poweres of particle-hole pairs in the interaction Hamiltonian. Appling the boson transformation method to the dynamical equation, we obtain the conventional dynamical equation in nonlinear lattices and another dynamical equation for a single quantum.[14] The bound states are obtained from the dynamical equation for a single quantum.

We start with the following model Hamiltonian:

$$H = \sum_{\mu,m} \hbar\omega_\mu b^\dagger_{\mu m} b_{\mu m} + \frac{1}{2}\int dxdy\psi^\dagger(x)\psi(x)V(x-y)\psi^\dagger(y)\psi(y), \tag{1}$$

An atom is well localized at the site m and feels an harmonic potential. $\hbar\omega_\mu$ is an eigenvalue of the atom in the harmonic potential. $b_{\mu m}$ is an annihilation operator of the atom with the eigenvalue $\hbar\omega_\mu$ at the site m. The second term on the right hand side of Eq.(1) is the interaction Hamiltonian denoted as H_I, in which nonlinearity is included. $V(x-y)$ is a two body potential. Then we put

$$\psi(x) = \sum_m \{w_0(x-R_m)b_{0m} + w_1(x-R_m)b_{1m} + \cdots\}, \tag{2}$$

where $w_\mu(x)$ is the wavefunction of an atom in the harmonic potential. The suffixes 0 and 1 mean the ground state and the first excited state, respectively. There is a relation between their wavefunctions:

$$w_1(x) = -2\zeta\nabla w_0(x), \qquad \zeta = \sqrt{\frac{\hbar}{2m\omega}}, \tag{3}$$

where ζ is a mean width of the zeropoint motion, m is the mass of an atom and ω is an eigenfrequency; $\omega_n = (n+\frac{1}{2})\omega$. Hereafter,we consider only the two levels; the ground state and the first excited state.

Now we investigate the number density operator $n(x)$. We can put

$$\psi^\dagger(x)\psi(x) = \sum_m \Big[w_0^2(x-R_m)b^\dagger_{0m}b_{0m} + w_1^2(x-R_m)b^\dagger_{1m}b_{1m} + \{c_1\frac{(-\zeta B_m\nabla)}{1!} + c_2\frac{(-\zeta B_m\nabla)^2}{2!} + c_3\frac{(-\zeta B_m\nabla)^3}{3!} + \cdots\}w_0^2(x-R_m)\Big] \tag{4}$$

where B_m is a phonon operator:

$$B_m \equiv b_{1m}^{\dagger} b_{0m} + b_{0m}^{\dagger} b_{1m}. \tag{5}$$

In Eq.(4) we include higher powers of the phonon operator B_m. This fact is justified as follows: i) Since atoms are well-localized, the width of energy bands of an atom $\Delta\epsilon$ is very much smaller than the eigenfrequency ω which is an energy difference between the two levels of the atom. $\Delta\epsilon$ is nearly equal to $1/T$, where T is a hopping time. ω is neary equal to $1/\tau$, where τ is a time of an up or down transition of an atom. In an interval T, many repetitions of the up and down transition can occur at the same site. Thus we can include higher powers of the phonon operator B_m. ii) The form of expansions in B_m is determined by the Ward-Takahashi relation. iii) Comparing the interaction Hamiltonian with the conventional nonlinear potential, we have $c_k = 1$ $(k = 1, 2, \cdots)$. In the interaction Hamiltonian H_I, we take into account only terms involved in particle-hole pairs. Thus we can write the ineraction Hamiltonian H_I as

$$H_I = \frac{1}{2} \sum_{m \neq n, \alpha\beta} \int dxdy \frac{(-\zeta B_m \nabla)^{\alpha}}{\alpha!} w_0^2(x - R_n) V(x - y) \frac{(-\zeta B_n \nabla)^{\beta}}{\beta!} w_0^2(y - R_n), \tag{6}$$

where $V_{(0n)}^{0n} = 0$ for n =odd number, because of symmetry of space inversion.

In order to obtain the dynamical equation for phonon operators $\{B_m\}$,we consider the internal freedom of a phonon operator $B_m(t)$ by introducing the time ordering operator and derive the equation of motion of the phonon operator. We make the random phase approximation and the nearest neighbour approximation. Using the gap equation obtained by the Ward-Takahashi relation, we obtain the Heisenberg equation for phonon operators $\{B_m\}$:

$$m \frac{d^2}{dt^2} B_m = -\phi'(B_m - B_{m-1}) + \phi'(B_{m+1} - B_m), \tag{7}$$

$$\phi(r) = \frac{U}{2} r^2 + \frac{V}{3} r^3 + \frac{W}{4} r^4 + \cdots. \tag{8}$$

Eq.(7) with eq.(8) is just like a dynamical equation for the displacement fields in the conventional nonlinear lattice theory, but we should note that $\{B_m\}$ are phonon operators.

Next we apply the boson transformation method to eq.(7) with (8). The boson transformed B_m is denoted by B_m^f, which satisfies eq.(7). We put

$$B_m^f = B_m^{(0)} + B_m^{(1)} + \cdots, \tag{9}$$

where $B_m^{(0)}$ is the ground state expectation value,$B_m^{(0)} =< 0|B_m^f|0 >$ and $B_m^{(1)}$ is a linear term of free phonon fields. If we make the tree approximation; all loop diagrams are disregarded, we obtain

$$m\frac{d^2B_m^{(0)}}{dt^2} = -\phi'(B_m^{(0)} - B_{m-1}^{(0)}) + \phi'(B_{m+1}^{(0)} - B_m^{(0)}), \tag{10}$$

$$m\frac{d^2B_m^{(1)}}{dt^2} - U(B_{m-1}^{(1)} + B_{m+1}^{(1)} - 2B_m^{(1)}) - \sum_n V_{mn}^{(1)}B_n^{(1)} = 0, \tag{11}$$

$$V_{mn}^{(1)} = \frac{\partial}{\partial B_m^{(0)}}\left[-\phi_N'(B_m^{(0)} - B_{m-1}^{(0)}) + \phi_N'(B_{m+1}^{(0)} - B_m^{(0)})\right], \tag{12}$$

where ϕ_N means the nonlinear potential in eq.(8). Eq.(10) is nothing but the dynamical equation for the displacement fields in the conventional nonlinear lattice theory. Eq.(11) determine the behaviour of a single quantum under the self-consistent potential (12) created by the extended objects $B_m^{(0)}$. There appear bound states of the physical quantum due to the self-consistent potential.

Now we investigate eqs.(10) and (11) with eq.(12) in the long wavelength limit. If we put $B_m^{(i)} = B^{(i)}(x,t), \quad x = ma$, we obtain

$$c_0^{-2}\varphi_{tt}^{(0)} - \varphi_{xx}^{(0)} - \frac{a^2}{12}\varphi_{xxxx}^{(0)} = \alpha\left(\varphi^{(0)^2}\right)_{xx} + \beta\left(\varphi^{(0)^3}\right)_{xx}, \tag{13}$$

$$c_0^{-2}\varphi_{tt}^{(1)} - \varphi_{xx}^{(1)} - \frac{a^2}{12}\varphi_{xxxx}^{(1)} = 2\alpha\left(\varphi^{(0)}\varphi^{(1)}\right)_{xx} + 3\beta\left(\varphi^{(0)^2}\varphi^{(1)}\right)_{xx}, \tag{14}$$

where

$$\varphi^{(i)}(x,t) = \frac{\partial B^{(i)}(x,t)}{\partial x}, \quad c_0^{-2} = \frac{m}{Ua^2}, \quad \alpha = \frac{aV}{U}, \quad \beta = \frac{a^2W}{U}. \tag{15}$$

Here a is an atomic distance. Eq.(13) is the Boussinesq equation which has soliton solutions:

$$\varphi^{(0)}(x,t) = \frac{k^2a^2}{2\alpha}\mathrm{sech}^2 k\xi \qquad (\frac{c}{c_0})^2 - 1 = \frac{(2ka)^2}{12}, \qquad \text{for cubic potential,} \tag{16}$$

$$\varphi^{(0)}(x,t) = \frac{ak}{\sqrt{6\beta}}\mathrm{sech}k\xi, \qquad (\frac{c}{c_0})^2 - 1 = \frac{(ak)^2}{12}, \qquad \text{for quartic potential,} \tag{17}$$

where $\xi = x - ct$ and k is a wavenumber. Eq.(14) determines the scattering states, the bound states and the translational modes with the self-consistent potential $\tilde{\varphi}(x) = 2\alpha\varphi^{(0)} = k^2a^2\mathrm{sech}^2 k\xi$ for cubic potential and $\tilde{\varphi}(x) = 3\beta\varphi^{(0)^2} = \frac{k^2a^2}{2}\mathrm{sech}^2 k\xi$ for quartic potential, respectively. Note that $\tilde{\varphi}$ does not depend on the coupling constants α and β.

We seek solutions to eq.(14) in the form:[15-18]

$$\varphi^{(1)}(x,t) = \cos(Kx - \Omega t)D(\xi). \tag{18}$$

Substituting eq.(18) into eq.(14), we obtain

$$\left[(\frac{c^2}{c_0^2} - 1)D - \frac{a^2}{12}D'' - \tilde{\varphi}D\right]'' - \left[(\frac{\Omega^2}{c_0^2K^2} - 1 + \frac{a^2K^2}{12})D - \frac{a^2}{2}D'' - \tilde{\varphi}D\right]K^2 = 0, \tag{19}$$

$$\left[(\frac{c\Omega}{c_0^2K} - 1 + \frac{a^2K^2}{6})D - \frac{a^2}{6}D'' - \tilde{\varphi}D\right]'K = 0. \tag{20}$$

In order to solve eqs.(19) and (20), we first consider the properties of eqs.(19) and (20). i)$K = 0, \Omega = 0$: the first bracket in eq.(19) remains. This equation has a solution $D(x) = \frac{d\varphi^{(0)}(x)}{dx}$, which is a translational mode. ii)$K \neq 0, \Omega \neq 0$: eq.(20) always holds. There exists a bound state, if a solution of eq.(20) is not orthogonal to a solution of eq.(19). iii)$K > k, \Omega > kc$: in eq.(19) the second bracket dominates. For all cases, these equations reduce to the Schrödinger equation:

$$D'' + U_0\mathrm{sech}^2 k\xi D + ED = 0. \tag{21}$$

If we put $u = \tanh k\xi$, eq.(21) leads to the associated Legendre differential equation:

$$\frac{d}{du}\left[(1-u^2)\frac{dD}{du}\right] + \left[\nu(\nu+1) - \frac{\mu^2}{1-u^2}\right]D = 0, \tag{22}$$

where $\mu^2 = -\frac{E}{k^2}$, $\nu(\nu+1) = \frac{U_0}{k^2}$. The solution finite for $u = 1$ is

$$D(u) = (1-u^2)^{\frac{\mu}{2}}F(\mu - \nu, \mu + \nu + 1, \mu + 1; \frac{1-u}{2}), \tag{23}$$

where F is the hypergeometric function. If D remains finite for $u = -1, \mu - \nu = -n$, where $n = 0, 1, 2, \cdots$; then F is a polynomial of degree n.

First, we investigate solutions for cubic pottential (α-term). i)$K = 0, \Omega = 0$. The translational mode comes from $\nu = 3; \mu =; D(\xi) = \mathrm{sech}^2 k\xi \tanh k\xi$. A bound state comes from : ii) $K \neq 0, \Omega \neq 0$. $\nu = 2; \mu = 2; D(\xi) = \mathrm{sech}^2 k\xi$, and iii)$K > k, \Omega > kc$. Eq.(19) leads to $\frac{U_0}{k^2} = 2 : \nu = 1; \mu = 1; D(\xi) = \mathrm{sech} k\xi$.

Next we investigate solutions for quartic potential (β-term). i) $K = 0, \Omega = 0$. The translational mode is $\nu = 2; \mu = 1; D(\xi) = \mathrm{sech} k\xi \tanh k\xi$. A bound state comes from : (ii)$K \neq 0, \Omega \neq 0$. $\nu = \frac{1}{2}(-1 + \sqrt{13}); \mu = \frac{1}{2}(-1 + \sqrt{13}); D(\xi) = (\mathrm{sech} k\xi)^{\frac{1}{2}(-1+\sqrt{13})}$, and iii)$K > k, \Omega > kc$. $\nu = \frac{1}{2}(-1 + \sqrt{5}), \mu = \frac{1}{2}(-1 + \sqrt{5}); D(\xi) = (\mathrm{sech} k\xi)^{\frac{1}{2}(-1+\sqrt{5})}$.

Takeno et al. have investigated the localized modes in the nonlinear dynamical equation (10). Our bound states come from the linear dynamical equation (11) with the potential (12) created by a soliton. The potential which a single quantum feels corresponds to the mean field in the nonlinear potential except factors 2 and 3 in front of α and β-terms in eq.(14). So the bound state can be regarded as the localized mode. Furthermore, in eq.(11) if the self-consistent potential $V_{mn}^{(1)}$ appears around a position, the situation corresponds to the increase of the elastic constant around the position in the classical lattice dynamics.[19,20] This causes the localized mode around the position. However, in lattices since the moving extended objects are not stable, the bound states or the localized modes are not stable in the longtime limit. In the longwavelenth limit, since there are stable solitons, the stable bound states or the localized modes can exist.

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